IV International Conference on Particle-based Methods – Fundamentals and Applications
PARTICLES 2015
E. Oñate, M. Bischoff, D.R.J. Owen, P. Wriggers & T. Zohdi (Eds)

BACK FROM THE SOLID TEMPERATURE TO KINETIC ENERGY OF ITS MACRO-MOLECULES

Sergey V. Arinchev

Moscow Bauman State Technical University
107005, 2-ya Baumanskaya street, 5/1, Moscow, Russian Federation
arinchev@inbox.ru

Key words: Solid, Macro-molecule, Temperature, Kinetic Energy

Summary. *For solving the solid heat-conduction problem, the "temperature" concept is replaced with the original "macro-molecule kinetic energy" concept. The heat-conduction problem is considered as the solid forced-vibration problem with the transient taken into account.*

The macro-molecules are point particles. Their contact is not available. Interaction of macro-molecules is determined by their force characteristic. Macro-molecule models of the solid bars made of different materials (steel, fluoroplastic, aluminium alloys) are tested for tension, compression and torsion in the laboratory [1-3] and proved their right of existence. For solving the test problems, the required number of macro-molecules is relatively small (about a hundred) and there is no need in a supercomputer.

The fact is that the available particle-based methods reveal the contradiction between their principle finite character and the classic continuous infinitesimal approach. For example, in the work [4] wee see the attempt to combine the finite particles and the point-stress concept. The work [5] presents the same attempt to combine the finite particles and the concepts of point temperature and point heat flux. There is even the attempt to approximate the 2^{nd}-order spatial derivative of the heat-conduction equation. Let's take another way. It is time to overcome the available indecision and hesitance and to meet the original discreet particle-based challenge. We know from the secondary school: there is no temperature, there is kinetic energy of separate molecules. So, using the well-known proportionality law

$$\overline{E} = \frac{3}{2}kT \qquad (1)$$

let us go right-to-left back home from the solid temperature to (averaged) kinetic energy of its macro-molecules.

It is better to take the relative values (2) to dispense with the dimensional quantities like

the Boltzmann conversion factor k. H_j is the j-th macro-molecule hotness degree, $j = 1,\ldots, n$.

$$\frac{T_j}{T_{\max}} = \frac{\overline{E}_j}{\overline{E}_{\max}} \approx \frac{H_j}{H_{\max}} \tag{2}$$

It is obtained by averaging (3) kinetic energy of the macro-molecule in the integration time interval t. The hotness-degree calculation procedure is specified below (see Figure 9).

$$H_j = \frac{\int_0^t E_j(\tau)d\tau}{t} \tag{3}$$

The considered 0.01×0.01×0.03 (m) solid bar is specified in Figure 1. The bar material

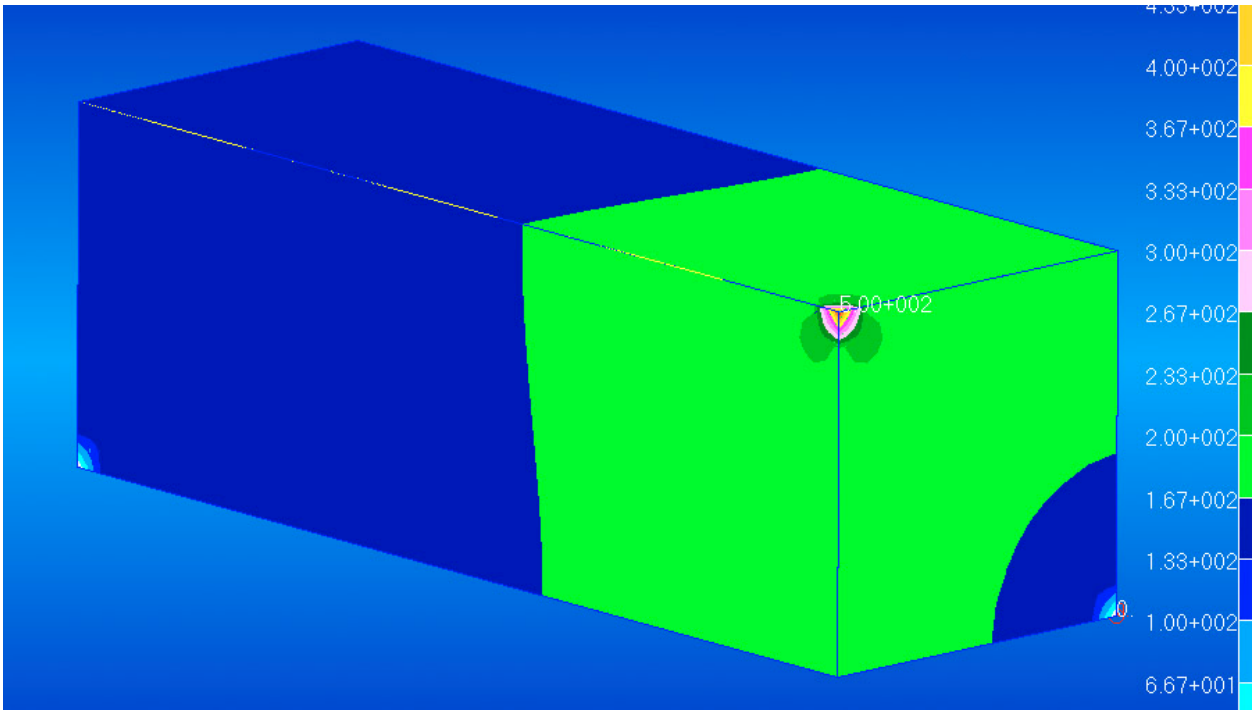

Figure 1: Bar reference temperature field (exact solution) obtained using MSC.Nastran.Thermal

is isotropic. The bar is loaded by applying the three point temperatures to its vertices: the two 0 ºK (frozen) vertices are in the bottom face, the 500 ºK (maximum temperature) vertex is in the front edge. Figure 1 presents the reference (exact) FEM solution of the steady-state heat-conduction problem obtained using MSC.Nastran.Thermal software. This exact temperature field is compared below with the determined distribution of the established macro-molecule hotness degree.

There are two important features of the obtained exact FEM solution:

1) **uniformity** of the temperature field. The colour change is available. But it is not a

temperature drop. It is just the vicinity of the (167 ºK) temperature-scale level specified in the Figure 1 right side. Except for the immediate loaded-vertex vicinity, the bar volume temperature varies by a dozen ºK. That is why the Figures below compare the exact FEM reference temperature distribution and the obtained macro-molecule hotness-degree distribution only 1) along the bar front upper edge (containing the maximum-temperature vertex) and 2) along the bar back lower edge (containing the frozen vertex). Approximate ratio of the bar volume temperature and the bar maximum temperature is 1/3. The ratio is 1.0 in the maximum-temperature point. It is 0.0 in the frozen point. The fact is that these values do not depend on the applied maximum temperature. It is the characteristic estimate of the (2) ratios.

2) **independence** of the obtained temperature field on thermal properties (specific heat, density, thermal conductivity factor) of the material. The fact is that the problem is a steady-state one, internal heat sources are not available, material is isotropic. So, the heat-conduction equation [5] is the homogeneous Laplace equation reduced by the temperature-conductivity factor. Likewise, this temperature field does not depend on mechanical properties (stiffness factor) of the material. So, the specified material properties of the macro-molecule model may be selected arbitrarily in compliance with the established calculation requirements.

The considered macro-molecule model is specified in Figure 2. It is developed using MSC.Adams software. The macro-molecules are arranged in the nodes of the design lattice.

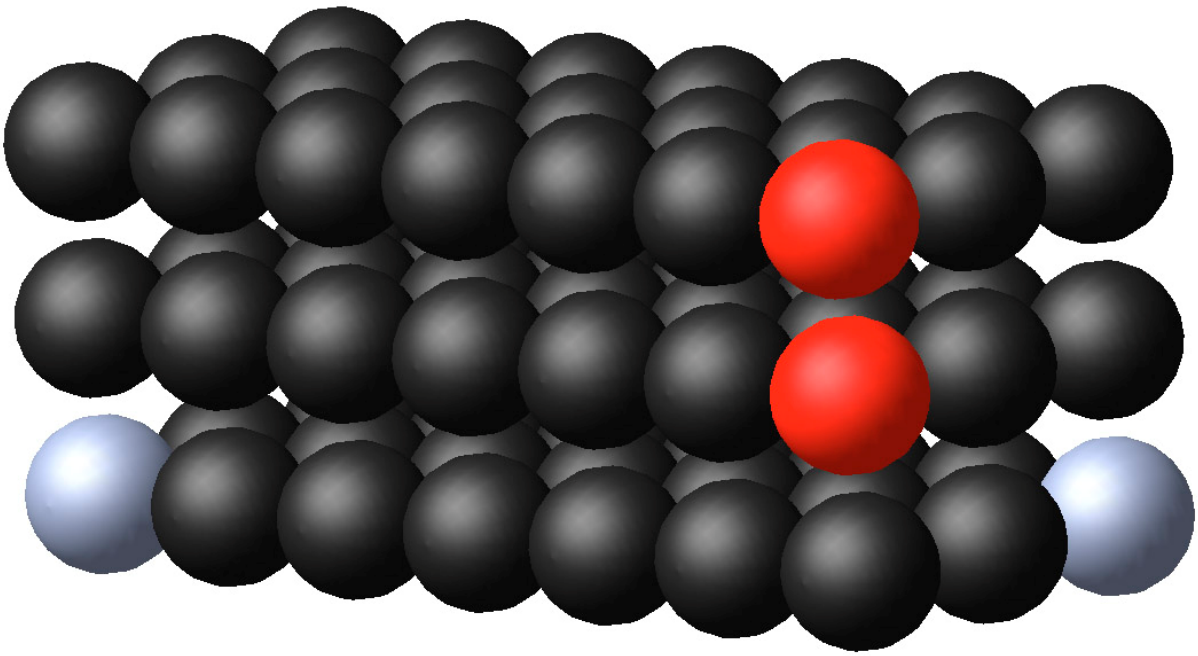

Figure 2: Bar macro-molecule model made of 3x3x7 = 63 molecules

Their interaction is determined by their force characteristic (specified below). If the macro-

molecule is hot, then it oscillates in the vicinity of its equilibrium state. The macro-molecules are fixed (slate-blue ones), if they are frozen. Heating load is applied to the two red points. It is the internal kinematic excitation. It means that these points move in relation to each other with the given intensity. This internal excitation may not be a noise one. Mono-harmonic excitation is sufficient. The 3D transient takes place. It finally converges to a steady-state kinetic-energy distribution. This distribution is compared with the exact FEM temperature field specified above.

It is important to trace convergence of the specified distribution in the model macro-molecule number. The bar edge ratio is 1:1:3. So, there are three options: 2x2x4 = 16 macro-molecules, 3x3x7 = 63 macro-molecules (see Figure 2) and 4x4x10 = 160 macro-molecules.

The main feature of the obtained exact FEM solution is distribution **uniformity**. The uniformity origin is understandable, if the particles contact with each other and exchange their impacts. But the macro-molecules do not contact with each other. They just oscillate in the vicinity of the lattice nodes. To solve the problem, let's consider the beam oscillation modes.

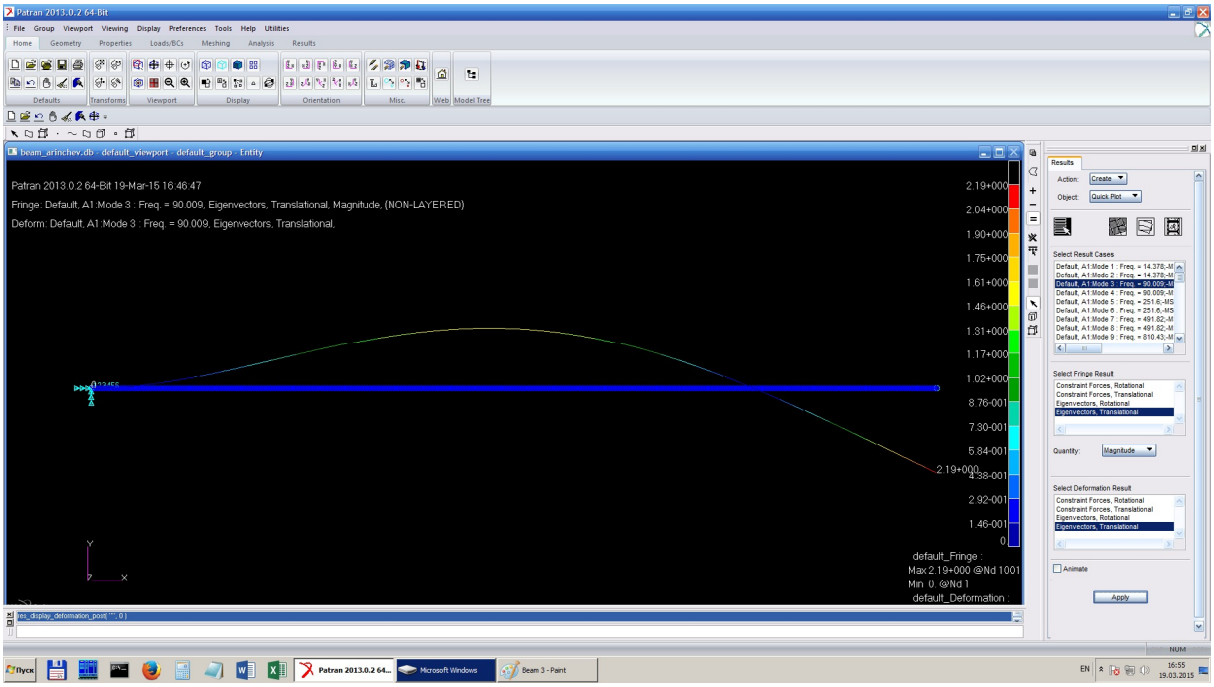

Figure 3: Beam oscillation mode No. 2

Figure 3 specifies the beam oscillation mode No. 2. Figure 4 specifies the beam oscillation mode No. 100. It is evident that the higher the mode No., the more uniform is the mode distribution. The conclusion is: only higher (molecular) harmonics shall be available in the heating excitation response. Lower harmonics (bending ones, torsion ones, tension ones, etc.) shall not be available. Figure 5 illustrates one of the bar lower bending oscillation modes. Figure 6 illustrates one of the bar higher molecular oscillation modes.

But there is the difficulty. Frequencies of the required molecular harmonics make hundreds

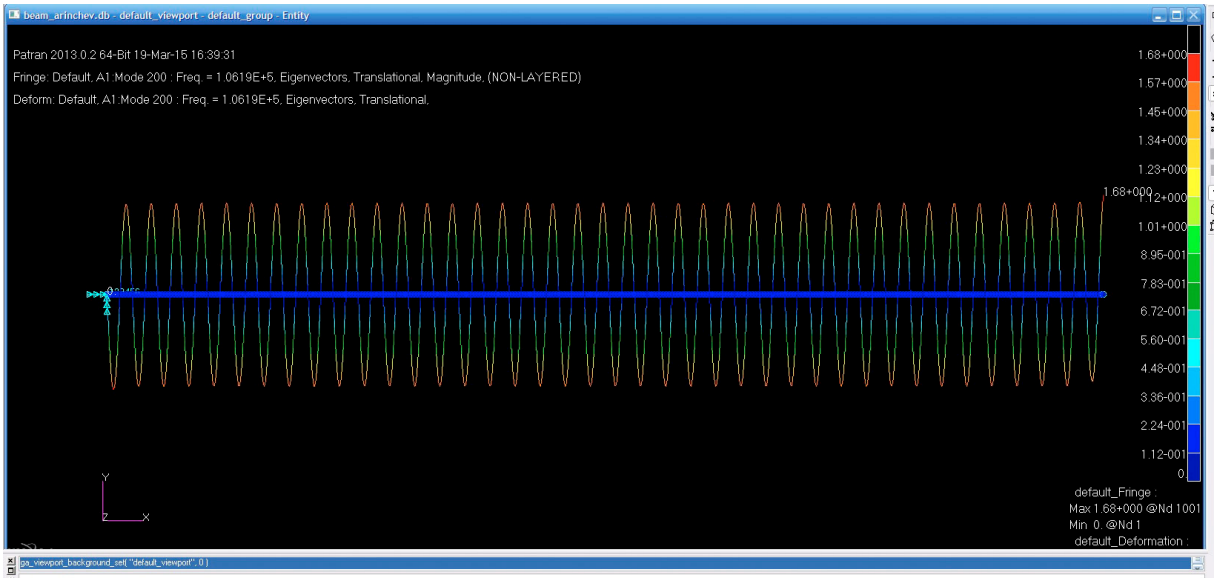

Figure 4: Beam oscillation mode No. 100

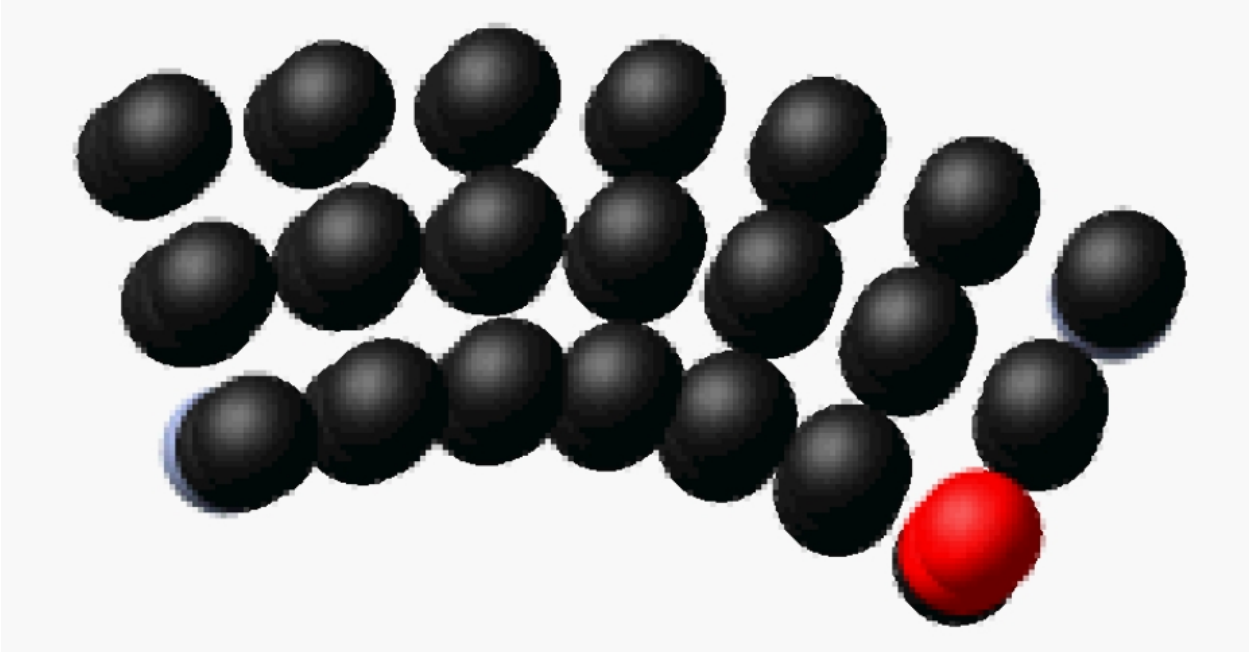

Figure 5: Bending oscillation mode of the bar made of 3x3x7=63 molecules (top view)

of thousands of Hz. It is really impossible to integrate such a transient. The outcome is to take into account the second important feature of the exact FEM solution: **independence** of the

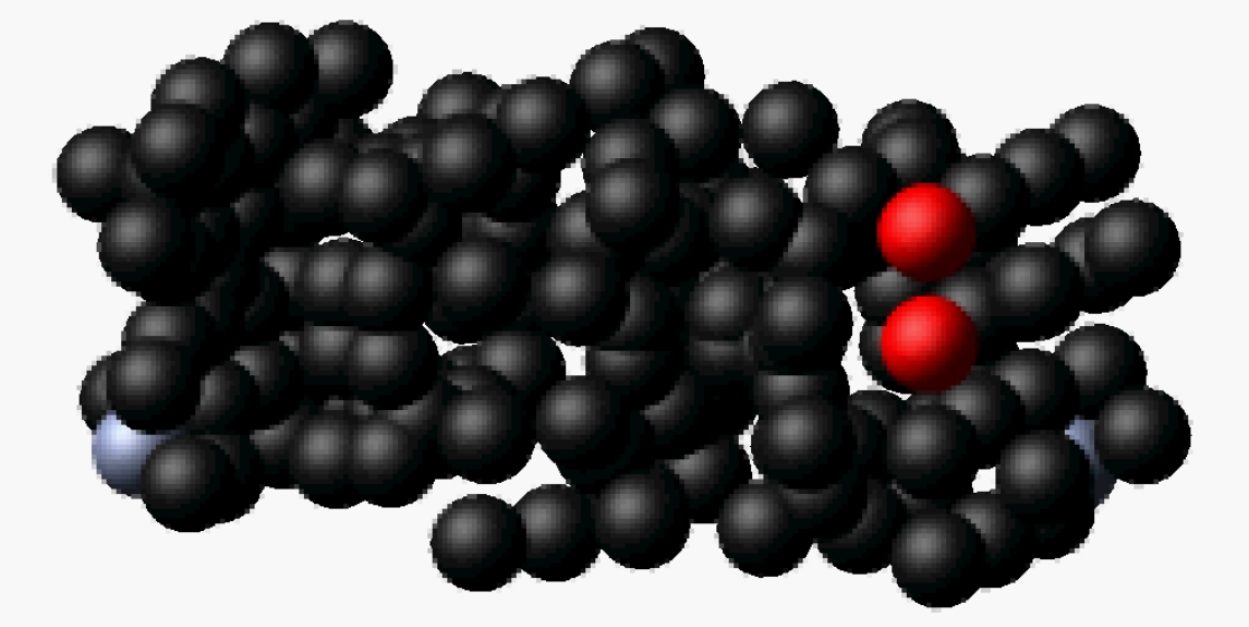

Figure 6: Molecular oscillation mode of the bar made of 4x4x10=160 molecules

solution on the material properties. So, let's lower the model stiffness factor (*A*, see below) to get down the available molecular frequency range and to provide the comfortable integration conditions. This assumption has the drawback. It makes impossible to solve the coupled problem of heat-conduction analysis and thermal-stress analysis at the same time for the same model. It is assumed that the comfortable upper frequency level is 50 Hz.

The macro-molecule interaction mode is "each one with each one except for itself". Interactions of the model containing 2x2x4 = 16 macro-molecules are illustrated in Figure 7 using thin lines in the MSC.Adams interface. The available number of combinations is significant. It requires developing a special program using the built-in MSC.Adams language.

The interactions are determined by the macro-molecule force characteristic. The macro-molecules are arranged in the lattice nodes. The material is an isotropic one, 3D central-symmetry interaction is available. There are many equilibrium positions. Potential of the Lennard-Jones type provides a single equilibrium position (root) and does not fit here. The multi-root macro-molecule force characteristic is developed in [2]. It is arranged within the envelope of the Lennard-Jones type. The required number of roots of the macro-molecule force characteristic is determined by the number of the macro-molecule essential neighbors specified in Figure 8. Let the red one be the given macro-molecule and the yellow ones be its neighbors. Let's assume that the force characteristic is set to zero, if the distance between the interacting macro-molecules exceeds 2*a*, where *a* is the lattice spacing parameter. (It is the so called short-range interaction and the most simple one.)

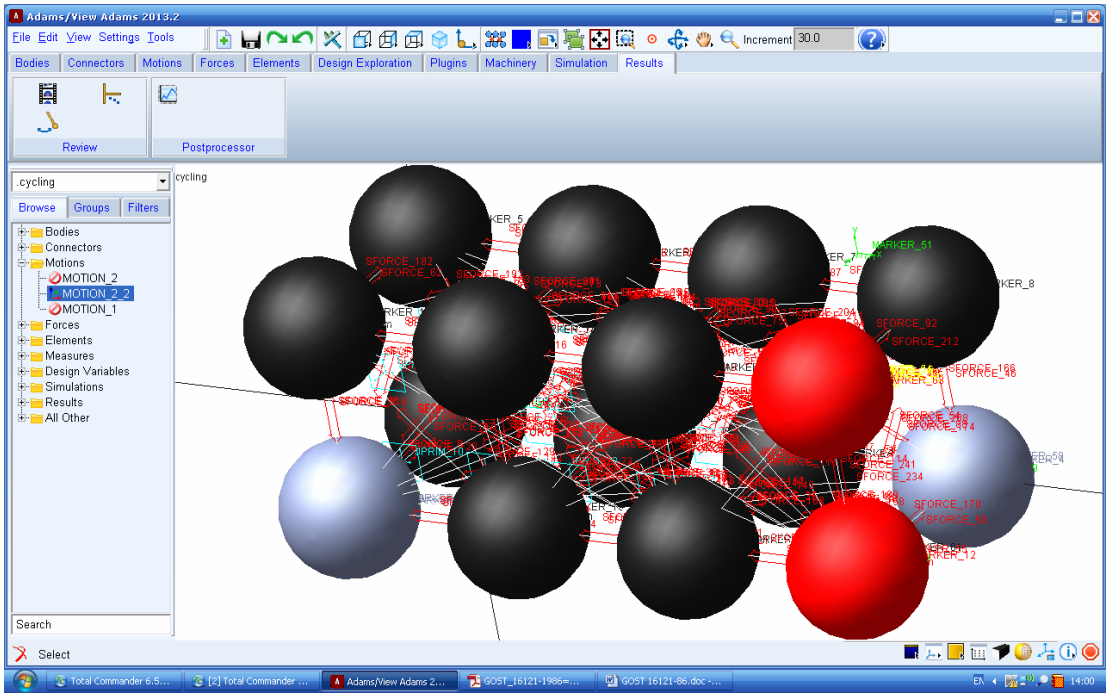

Figure 7: Bar macro-molecular model made of 2x2x4= 16 molecules in MSC.Adams

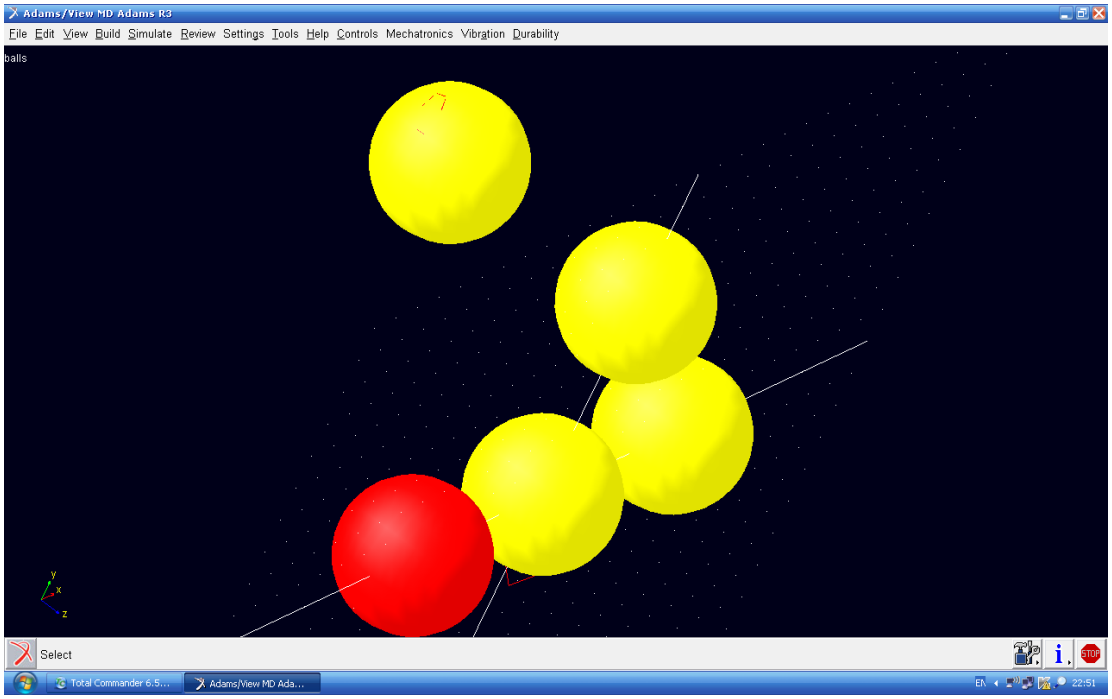

Figure 8: Four essential neighbors (yellow) of the given macro-molecule (red)

In this case, all the neighboring interacting macro-molecules may be subdivided into four groups. Within each group, distance between the given (red) macro-molecule and the selected group member is the same. So, the whole group of the neighboring macro-molecules may be represented by a one of them. This is the essential neighbor. Figure 8 presents four essential neighbors. So, at least four roots shall be available in the macro-molecule force characteristic.

But that is not all. The required equilibrium state shall not be just available. It shall be stable as well, and derivative of the force-characteristic curve shall be positive in the equilibrium point. To obtain the positive derivatives in the two neighboring roots, the curve shall go up, then go down and then again go up between them. That is why, an additional root between each pair of the specified ones takes place, and the following seven-root force characteristic is taken into account for the short-range macro-molecule interaction [2]:

$$F_{jk}(r_{jk},\dot{r}_{jk}) = A(r_{jk}-a_1)^p[\prod_{i=1}^{7}(r_{jk}-a_i)]step(r_{jk},2sa,1.0,2a,0.0)+\delta\dot{r}_{jk} \qquad (4)$$

where:
F_{jk} – interaction force between the j-th and the k-th macro-molecules;
r_{jk} - distance between the j-th and the k-th macro-molecules;
$\dot{r}_{jk}$ - relative radial velocity of the j-th and the k-th macro-molecules;
A – stiffness factor;
a_i, i = 1,…,7 – seven roots of the force-characteristic curve;
p – exponent of the increasing component of the curve envelope;
step(…) – standard (cubic-parabola) function of the built-in MSC.Adams view-command language (decreasing component of the curve envelope);
s – decrease factor of the curve envelope;
a – lattice spacing parameter;
δ – damping factor.

Formula (4) has two components: positional component with the stiffness factor A and the damping component with the damping factor δ. A is the factor that shall be lowered (see above) to get down the available molecular frequency range and to provide the comfortable integration conditions. δ is the factor providing numerical stability of the available integration procedure. It may affect the obtained solution of the considered heat-conduction problem.

Thermo-dynamic equations of the considered macro-molecule model (5) are dynamic

$$-m_j\ddot{\bar{r}}_j-\sum_{\substack{k=1\\k\neq j}}^{n}\bar{F}_{jk}=0 \quad ,j=1,\ldots,n \qquad (5)$$

equations for point masses m_j. The equations include inertia forces and the interaction forces between macro-molecules determined by their force characteristic (4). Rotations are forbidden. If time $\tau = 0$, then the entire model rests (is frozen). Two molecules (see slate-blue ones in Figure 2) remain frozen during the entire integration process in compliance with the imposed freezing conditions:

$$\bar{r}_i = \bar{r}_{i0} \;;\; \bar{r}_l = \bar{r}_{l0} \tag{6}$$

The red molecules (see Figure 2) move in relation to each other in the vertical direction in compliance with the imposed heating conditions:

$$(\bar{r}_m - \bar{r}_q) \cdot \bar{e}_2 = a + D\sin(2\pi f \tau) \tag{7}$$

where:
a – lattice spacing parameter;
$\bar{e}_2$ - unit vector of the vertical (Y-coordinate) axis;
D – heating excitation intensity (not exceeding $0.1a$);
f – heating excitation frequency (is selected arbitrarily in the 50 Hz vicinity).
So, the problem of the solid heat conduction is reduced to the problem of forced vibrations of the system of point masses with the transient taken into account. In this system the temperature concept is replaced with the concept of the macro-molecule hotness degree.

Figure 9 specifies the hotness-degree calculation procedure in compliance with formula (3). The red curve is kinetic energy of the macro-molecule No. 157 depending on time τ.

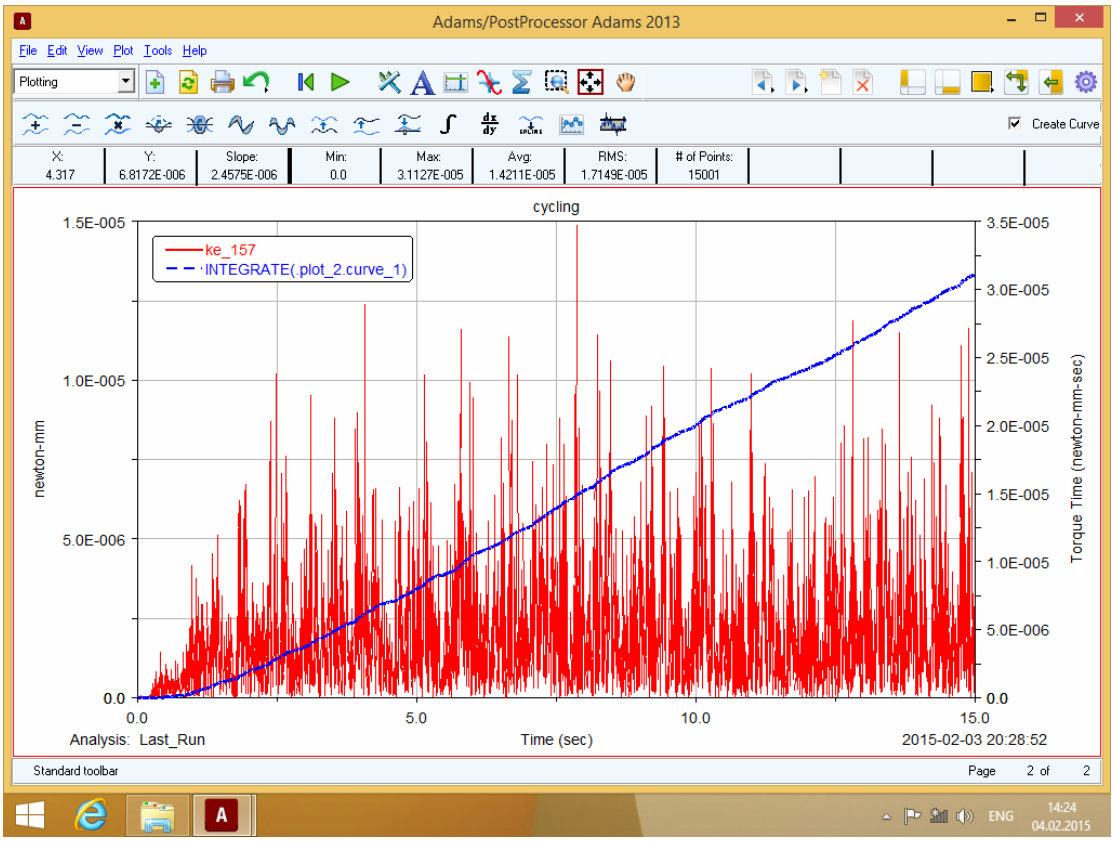

Figure 9: Macro-molecule hotness-degree calculation procedure

Heating excitation is mono-harmonic (7). But the response is a poly-harmonic one. Integration time interval is t = 15 s. It is long enough to cope with the transient and to obtain the steady-state process. The blue curve is the integral substituted in the numerator of the fraction (3). This integral is close to a straight line denoting that the steady-state heating process is obtained.

The Figures 10-12 present the obtained calculation results. They characterize the macro-molecule hotness degree distribution within the solid bar. This distribution has the uniform character. That is why the results specify only the upper front edge of the bar (see Figures 1-2) and its lower back edge. Convergence in the number of molecules is important. That is why there are three options: 16 molecules (Figure 10), 63 molecules (Figure 11) and 160 molecules (Figure 12). Damping factor δ is varied approximately two times in the vicinity of the obtained solution. Red continuous lines specify the exact finite-element relative-temperature (2) solution obtained using MSC.Nastran.Thermal software (see Figure 1). Polylines specify the corresponding macro-molecule approach using relative hotness degree. There are 4 macro-molecules in the Figure 7 edge. That is why there are four vertices in the

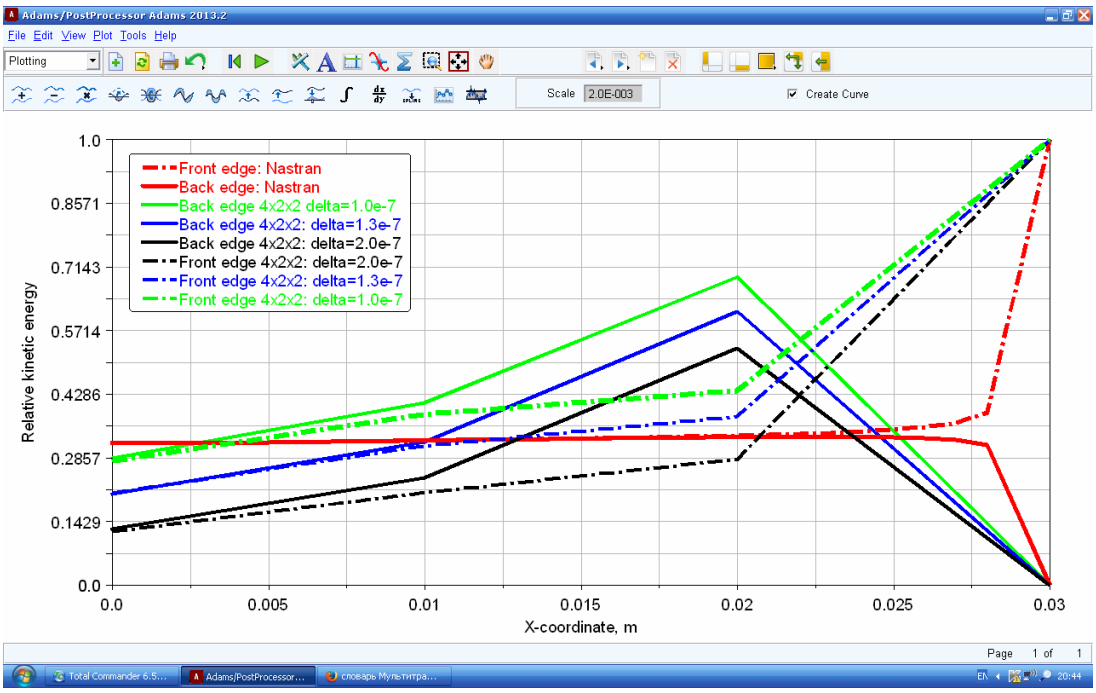

Figure 10: Macro-molecule relative hotness degree
distributed along the edges of the model made of 2x2x4=16 molecules

Figure 10 polyline. The dash-dot lines refer to the upper front edge. The solid lines refer to the lower back edge.

It is evident that the obtained macro-molecule result and the exact finite-element result are sufficiently close to each other. The higher the number of macro-molecules of the considered model, the smoother the polylines, the lower the influence of the damping factor.

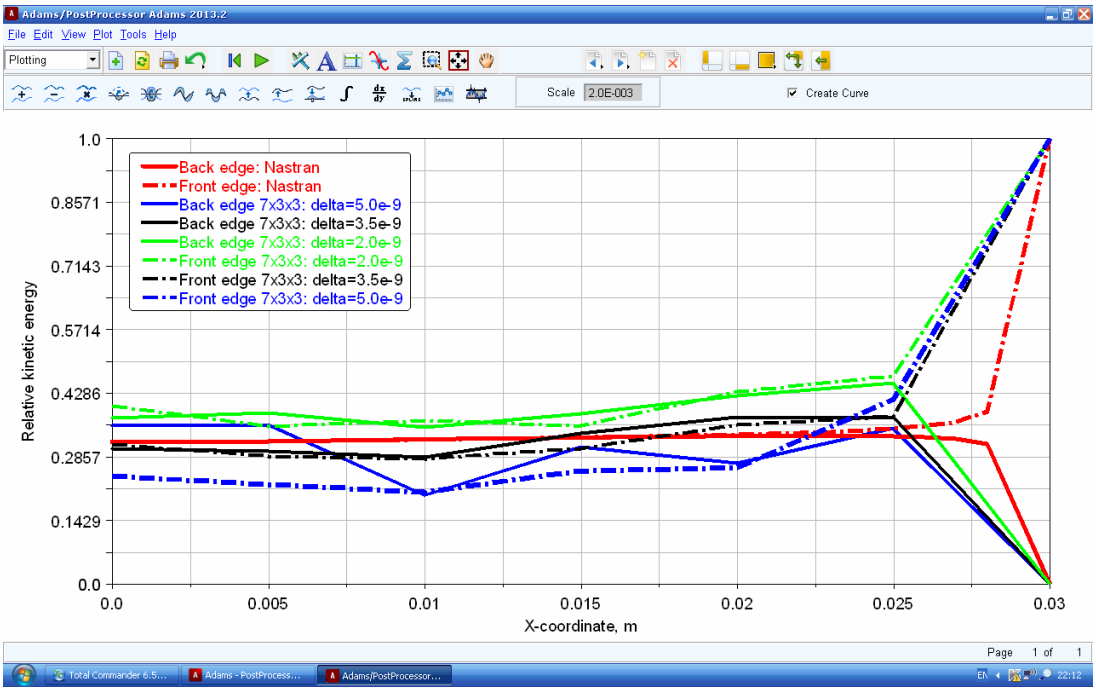

Figure 11: Macro-molecule relative hotness degree
distributed along the edges of the model made of 3x3x7=63 molecules

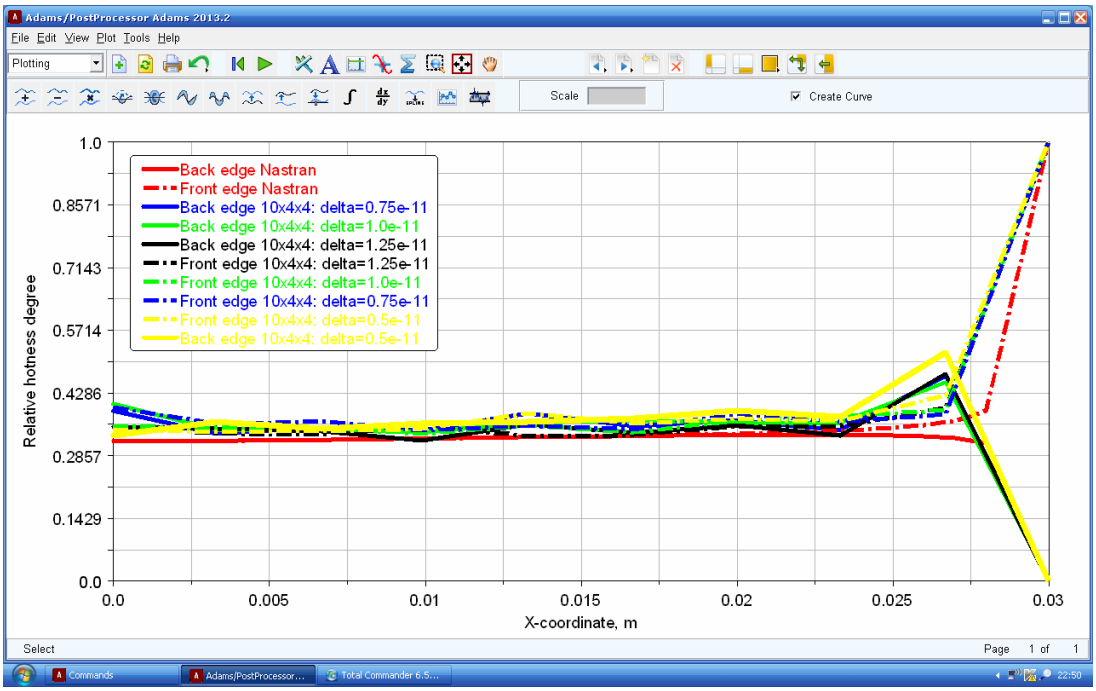

Figure 12: Macro-molecule relative hotness degree
distributed along the edges of the model made of 4x4x10=160 molecules

CONCLUSIONS

- Solution of the considered heat-conduction problem may be obtained by replacing the concept of temperature with the original “macro-molecule kinetic energy” concept.
- The approach has a drawback: it can not be used for solving the coupled problem of heat-conduction analysis and thermal-stress analysis at the same time for the same model.

REFERENCES

[1] Аринчев С.В., Yuri Sillano. Моделирование процесса разрыва стального бруск методом частиц в среде MSC.Adams // *Russian Federation, Известия ВУЗов Машиностроение* (2012)**6**:39-45.

[2] Sergey V. Arinchev. Simulation of high-ratio compression of a parallelepipedal duralumin bar using the particle-based method and MSC.Adams software // *CIMNE. Proceedings of the III International Conference on Particle-based methods. – Fundamentals and Applications. University of Stuttgart (Germany), 2013, 18-20 September, Ebook: p.* 670-680.

[3] Аринчев С.В., Букеткин Б.В. Моделирование процесса кручения стержня из фторопласта методом «частиц» // *Russian Federation, Известия ВУЗов, Машиностроение* (2014)**4**:38-43.

[4] Fabian Spreng, Alexandra Mueller and Peter Eberhard. The introduction of a bi-adaptive smoothed particle hydrodynamics formulation beneficial for machining process simulation // *CIMNE. Proceedings of the III International Conference on Particle-based methods. – Fundamentals and Applications. University of Stuttgart (Germany), 2013, 18-20 September, Ebook*: p. 602-613.

[5] Patrick H. Peacock, David W. Holmes Development and verification of a particle number density variant of SPH to robustly incorporate energy and heat transfer // *CIMNE. Proceedings of the III International Conference on Particle-based methods. – Fundamentals and Applications. University of Stuttgart (Germany), 2013, 18-20 September, Ebook*: p. 949-960.